Stationary states of the Gross-Pitaevskii equation with linear counterpart

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Abstract

We study the stationary solutions of the Gross-Pitaevskii equation that reduce, in the limit of vanishing non-linearity, to the eigenfunctions of the associated Schrödinger equation. By providing analytical and numerical support, we conjecture an existence condition for these solutions in terms of the ratio between their proper frequency (chemical potential) and the corresponding linear eigenvalue. We also give approximate expressions for the stationary solutions which become exact in the opposite limit of strong non-linearity. For one-dimensional systems these solutions have the form of a chain of dark or bright solitons depending on the sign of the non-linearity. We demonstrate that in the case of negative non-linearity (attractive interaction) the norm of the solutions is always bounded for dimensions greater than one.

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1 Introduction

Recent achievement of Bose-Einstein condensation (BEC) in gases of alkali atoms has generated an impressive amount of experimental and theoretical works [1, 2]. In these systems the condensate is usually described by the so-called Gross-Pitaevskii equation (GPE), a Schrödinger equation with a local

cubic non-linear term which represents the interaction among the bosons in a mean field approximation. GPE effectively reproduces the ground state properties of a condensed boson gas confined by an external potential at zero temperature [2]. In the framework of linear response theory, the mean field approximation also allows to evaluate the spectrum of the excitations in presence of an external time-dependent perturbation [3, 4]. On the other hand, GPE also appears in the description of other physical systems, like nonlinear optics [5], molecular physics [6], *etc.*.

In this paper we study general properties of the stationary solutions of GPE both in the case of repulsive and attractive interaction. Besides its mathematical interest, this study is relevant in the search of the so-called vortex states and, in general, in understanding the dynamical properties of condensates. We choose to work in the grand-canonical ensemble, that is we fix the chemical potential μ of the system, *i.e.* the proper frequency for the time evolution, and derive the number of particles corresponding to each stationary solution. In particular, we study the stationary solutions of GPE that have a linear counterpart, in the sense that they reduce to the eigenstates of the linear Schrödinger equation which is the limit of GPE for vanishing interaction. For these states we conjecture an existence condition which depend on the ratio between the chemical potential and the corresponding eigenvalue of the associated Schrödinger equation. We give a proof of this conjecture for the node-less state of a system in presence of a general external potential and verify it for the exactly solvable case of a one-dimensional, infinitely deep, square well. We also provide numerical evidence of the validity of the conjecture by studying systems with harmonic potentials in different dimensions.

As a consequence of the above conjecture, we find that in the case of attractive condensates there exists a range of the chemical potential μ in which the node-less stationary solution does not exist and the lowest-energy state has one or more nodes. This may be relevant for the observation of stable vortex states.

We also study the limit of strong non-linearity of GPE obtained for large values of the modulus of the chemical potential μ. In this limit a Thomas-Fermi approximation holds for repulsive systems, while for attractive systems the solutions become independent of the external potential. In the one-dimensional case the corresponding approximate solutions have the form of a chain of dark or bright solitons depending on the sign of the non-linearity. We use these asymptotically exact expressions to establish that the number of particles in the ground state of an attractive condensate is always bounded for dimensions greater than one in agreement with previous numerical results [7].

2 The linear limit

We consider the Gross-Pitaevskii equation [8, 9] describing, in the mean field approximation, a system of interacting particles confined by an external potential $V(\boldsymbol{x})$

$$i\hbar\frac{\partial\Psi(\boldsymbol{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\boldsymbol{x},t) + U_0|\Psi(\boldsymbol{x},t)|^2\Psi(\boldsymbol{x},t) + V(\boldsymbol{x})\Psi(\boldsymbol{x},t), \tag{1}$$

with $\boldsymbol{x} \in \mathbb{R}^d$. The constant U_0 is positive (negative) in the case of repulsive (attractive) interaction. Equation (1) has two conserved quantities, namely the number of particles (squared norm)

$$N[\Psi] = \int |\Psi(\boldsymbol{x},t)|^2 d\boldsymbol{x} \tag{2}$$

and the energy

$$E[\Psi] = \int \left[\frac{\hbar^2}{2m}|\nabla\Psi(\boldsymbol{x},t)|^2 + \frac{U_0}{2}|\Psi(\boldsymbol{x},t)|^4 + V(\boldsymbol{x})|\Psi(\boldsymbol{x},t)|^2\right] d\boldsymbol{x}. \tag{3}$$

The stationary states of Eq. (1), $\Psi(\boldsymbol{x},t) = \exp\left(-\frac{i}{\hbar}\mu t\right)\psi(\boldsymbol{x})$, where μ is the chemical potential are determined by the equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x}) + U_0|\psi(\boldsymbol{x})|^2\psi(\boldsymbol{x}) + V(\boldsymbol{x})\psi(\boldsymbol{x}) - \mu\psi(\boldsymbol{x}) = 0, \tag{4}$$

i.e. as critical points of the grand-potential functional

$$\begin{aligned}\Omega[\psi] &= \int \left[\frac{\hbar^2}{2m}|\nabla\psi(\boldsymbol{x})|^2 + \frac{U_0}{2}|\psi(\boldsymbol{x})|^4 + (V(\boldsymbol{x}) - \mu)\,|\psi(\boldsymbol{x})|^2\right] d\boldsymbol{x} \\ &= E[\psi] - \mu N[\psi].\end{aligned} \tag{5}$$

It is simple to show [10] that if ψ is a solution of (4) then

$$\Omega[\psi] = -\frac{U_0}{2}\int |\psi(\boldsymbol{x})|^4 d\boldsymbol{x}. \tag{6}$$

We will look for the solutions of (4) corresponding to a given chemical potential μ. In this paper, we concentrate on solutions which admit a linear counterpart in the sense that they reduce, in a proper limit, to the eigenfunctions of the associated linear problem

$$-\frac{\hbar^2}{2m}\nabla^2\phi_n(\boldsymbol{x}) + V(\boldsymbol{x})\phi_n(\boldsymbol{x}) - \mathcal{E}_n\phi_n(\boldsymbol{x}) = 0. \tag{7}$$

Here we suppose that $\mathcal{E}_0 \leq \mathcal{E}_1 \leq \ldots \leq \mathcal{E}_n$ and $\{\phi_n(\boldsymbol{x})\}$ is a hortonormal base with $\phi_0(\boldsymbol{x})$ positive and bounded. Solutions without linear counterpart will be discussed in another paper [11].

By substituting $\psi(\boldsymbol{x}) = \sqrt{N(\mu)}\chi(\boldsymbol{x})$ in (4) with $||\chi|| = 1$, we have

$$-\frac{\hbar^2}{2m}\nabla^2\chi(\boldsymbol{x}) + U_0 N(\mu)|\chi(\boldsymbol{x})|^2\chi(\boldsymbol{x}) + (V(\boldsymbol{x}) - \mu)\chi(\boldsymbol{x}) = 0. \tag{8}$$

If the number of particles is sufficiently small, the nonlinear term in (8) can be neglected and χ approximated by ϕ_n. By substituting χ with ϕ_n, Eq. (8) provides the following relation between the chemical potential μ and the corresponding norm $N(\mu)$

$$\mu \simeq \mathcal{E}_n + U_0 N(\mu)||\phi_n^2||^2. \tag{9}$$

Equation (9) suggests the following conjecture for the existence of solutions of (4) with linear counterpart

Conjecture. *For $U_0 > 0$ ($U_0 < 0$), solutions with linear limit $\psi \simeq \sqrt{N(\mu)}\phi_n$ exist only if $\mu > \mathcal{E}_n$ ($\mu < \mathcal{E}_n$). Moreover $N(\mu) \to 0$ for $\mu \to \mathcal{E}_n$.*

In Appendix A we give a general proof of this conjecture in the case $n = 0$.

The conjecture can be verified analytically in the case of a 1-dimensional system confined in a box of size L, i.e. with

$$V(x) = \begin{cases} 0 & |x| < L/2 \\ \infty & |x| > L/2 \end{cases}. \tag{10}$$

For this problem the solutions of (4) are known [12]. In the case $U_0 > 0$ they are given by the Jacobi elliptic functions

$$\psi_n(x) = A \; \mathrm{sn}\left(2(n+1)\mathrm{K}(p)\left(\frac{x}{L} + \frac{1}{2}\right) \middle| \, p \right), \tag{11}$$

where

$$\mathrm{K}(p) = \int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1 - p\sin^2\theta}} d\theta \tag{12}$$

is the complete elliptic integral of the first kind with modulus $p \in [0, 1]$, and $n = 0, 1, 2, \ldots$. By substituting (11) into (4), one finds the conditions

$$A^2 = \frac{\hbar^2}{mU_0L^2} \, p \, (2(n+1)\mathrm{K}(p))^2, \tag{13}$$

$$\mu = \frac{\hbar^2}{mL^2} \frac{p+1}{2} \, (2(n+1)\mathrm{K}(p))^2. \tag{14}$$

The number of particles and the energy are given by

$$N(\mu) = \frac{\hbar^2}{mU_0 L} \, (2(n+1)\mathrm{K}(p))^2 \left(1 - \frac{\mathrm{E}(p)}{\mathrm{K}(p)}\right), \tag{15}$$

$$E(\mu) = N\mathcal{E}_0 \, \frac{(n+1)^2}{3} \left(\frac{2\mathrm{K}(p)}{\pi}\right)^2 \, \frac{p + (p+1)\left(1 - \frac{\mathrm{E}(p)}{\mathrm{K}(p)}\right)}{1 - \frac{\mathrm{E}(p)}{\mathrm{K}(p)}}, \tag{16}$$

where

$$\mathrm{E}(p) = \int_0^{\frac{\pi}{2}} \sqrt{1 - p\sin^2\theta} \; d\theta \tag{17}$$

is the complete elliptic integral of the second kind with p determined in terms of μ by Eq. (14). Since $\mathrm{K}(p)$ increases monotonously from $\mathrm{K}(0) = \pi/2$, for a given n Eq. (14) has solution only if

$$\mu \geq \mathcal{E}_n \equiv \frac{(n+1)^2\pi^2\hbar^2}{2mL^2} \tag{18}$$

which complies with the conjecture formulated above. The same conclusion can also be reached by using the theorems of [10].

In the linear limit $\mu \to \mathcal{E}_n$, the solutions (11) reduce to the eigenfunctions of the associated Schrödinger equation

$$\frac{1}{\sqrt{N(\mu)}}\psi_n(x) \stackrel{\mu\to\mathcal{E}_n}{\longrightarrow} \sqrt{\frac{2}{L}} \sin\left[\left(\frac{x}{L} + \frac{1}{2}\right)(n+1)\pi\right]. \tag{19}$$

In the opposite limit of strong nonlinearity, $\mu \gg \mathcal{E}_n$, we get from (11) the dark soliton solutions

$$\psi_n(x) \stackrel{\mu\gg\mathcal{E}_n}{\longrightarrow} \sqrt{\frac{\mu}{U_0}} \prod_{k=0}^{n+1} \tanh\left(\frac{\sqrt{m\mu}}{\hbar}(x - x_k)\right), \tag{20}$$

$$x_k = -\frac{L}{2} + \frac{L}{n+1}k. \tag{21}$$

Similar results are obtained in the case $U_0 < 0$. The solutions of (4) are now given by

$$\psi(x) = A \;\mathrm{cn}\left(2(n+1)\mathrm{K}(p)\left(\frac{x}{L} + \frac{1}{2}\right) + \mathrm{K}(p)\middle|\, p\right) \tag{22}$$

with the conditions

$$A^2 = -\frac{\hbar^2}{mU_0L^2}\, p\, (2(n+1)\mathrm{K}(p))^2 \tag{23}$$

$$\mu = \frac{\hbar^2}{mL^2}\,\frac{1-2p}{2}\,(2(n+1)\mathrm{K}(p))^2. \tag{24}$$

Number of particles and the energy become

$$N(\mu) = -\frac{\hbar^2}{mU_0L}\,(2(n+1)\mathrm{K}(p))^2\left(p-1+\frac{\mathrm{E}(p)}{\mathrm{K}(p)}\right), \tag{25}$$

$$E(\mu) = N\mathcal{E}_0\,\frac{(n+1)^2}{3}\left(\frac{2\mathrm{K}(p)}{\pi}\right)^2\,\frac{p(1-p)+(1-2p)\left(p-1+\frac{\mathrm{E}(p)}{\mathrm{K}(p)}\right)}{p-1+\frac{\mathrm{E}(p)}{\mathrm{K}(p)}}, \tag{26}$$

where p is determined by Eq. (24). Since $(1-2p)\mathrm{K}(p)$ decreases monotonously for $p\in[0,1]$, the n-node solution exists only if $\mu\le\mathcal{E}_n$ as conjectured above.

For $\mu\to\mathcal{E}_n$ the solutions (22) have the same limit (19). For $-\mu\gg\mathcal{E}_n$, we get the bright soliton solutions

$$\psi_n(x) \quad \xrightarrow{-\mu\gg\mathcal{E}_n} \quad \sqrt{\frac{2\mu}{U_0}}\,\sum_{k=0}^{n}(-1)^k\mathrm{sech}\left(\frac{\sqrt{-2m\mu}}{\hbar}(x-x_k)\right), \tag{27}$$

$$x_k = -\frac{L}{2}+\frac{L}{n+1}\left(k+\frac{1}{2}\right). \tag{28}$$

In Fig. 1 we show the behaviour of $N(\mu)$ evaluated according to (15) and (25) for the states $n=0$ and $n=1$. Note that $N(\mu)\to 0$ for $\mu\to\mathcal{E}_n$. The single-particle energy, $E(\mu)/N(\mu)$, for the same states is shown in Fig. 2

We have verified the above conjecture with numerical and analytical methods also in the case of a quadratic potential $V(\boldsymbol{x})=\frac{1}{2}m\omega^2\sum_{i=1}^{d}x_i^2$, with $d=1,2,3$. For example, in the case $d=1$ consider the following Ansatz for the solutions of (4)

$$\psi_n(x) = a_n\,\exp\left(-\frac{x^2}{2b_n^2}\right)H_n\left(\frac{x}{b_n}\right), \tag{29}$$

where $H_n(x)$ is the Hermite polynomial of degree n and a_n, b_n are real constants. Extremization of the functional Ω with respect to a_n and b_n leads

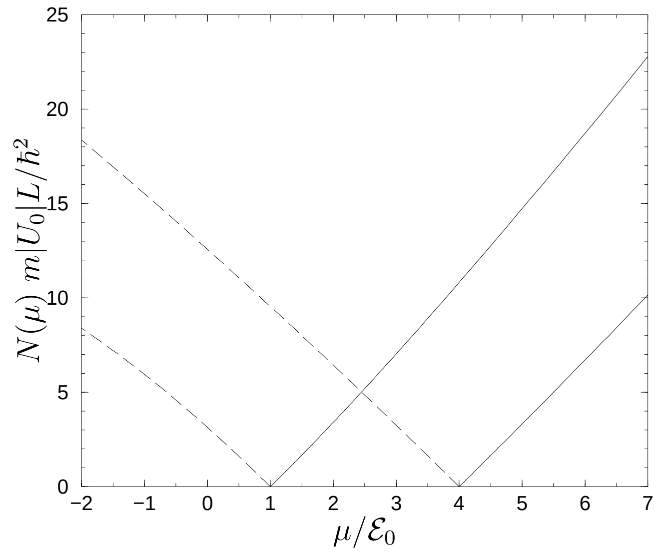

Figure 1: Number of particles N as a function of the chemical potential μ for the one dimensional square well. The solid and dashed lines are given by Eqs. (15) and (25), respectively. The two curves correspond to the states $n = 0$ and $n = 1$.

to

$$a_n^2 = \frac{\mu}{U_0}\,\frac{2^{n+1}n!\left(8-\sqrt{4+15(2n+1)^2\eta^2}\right)}{15 g_n}, \tag{30}$$

$$b_n^2 = \frac{\hbar^2}{m\mu}\,\frac{2+\sqrt{4+15(2n+1)^2\eta^2}}{5(2n+1)\eta}, \tag{31}$$

where $\eta = \hbar^2\omega^2/\mu^2$ and $g_n = \int_{-\infty}^{\infty} H_n(x)^4 dx$. If $U_0 > 0$, the condition $a_n^2 > 0$ implies $\mu > \left(n+\frac{1}{2}\right)\hbar\omega$. If $U_0 < 0$, the same condition leads to $\mu < \left(n+\frac{1}{2}\right)\hbar\omega$. Note that in the linear limit $\mu \to (n+\frac{1}{2})\hbar\omega$, we have $N \propto a_n^2 \to 0$ and $b_n^2 \to \hbar/m\omega$.

Analogously, in the case $d = 2$ consider the Ansatz

$$\psi_n(x_1,x_2) = a_n\ \exp\left(-\frac{x^2}{2b_n^2}\right) F\left(-n, |m|+1, \left(\frac{r}{b_n}\right)\right)\left(\frac{r}{b_n}\right)^{|m|} e^{im\theta}, \tag{32}$$

where $r^2 = x_1^2 + x_2^2$, $\tan\theta = x_2/x_1$ and $F(n,m,r)$ is the confluent hypergeometric function [13]. The condition $a_n^2 > 0$ is now equivalent to $\mu > \mathcal{E}_{n,m}$ if $U_0 > 0$, and $\mu < \mathcal{E}_{n,m}$ if $U_0 < 0$, where $\mathcal{E}_{n,m} = (2n + |m| + 1)\,\hbar\omega$ are the eigenvalues of the associated Schrödinger equation.

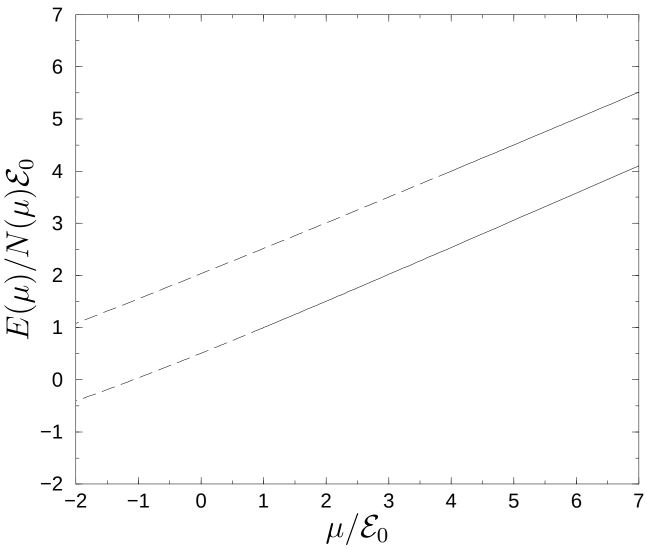

Figure 2: Single-particle energy E/N as a function of the chemical potential μ for the same states of Fig. 1. The solid and dashed lines are given by Eqs. (16) and (26), respectively.

Equation (4) has also been solved numerically with a standard relaxation algorithm [14]. In Fig. 3 we show the number of particles obtained as a function of the chemical potential μ for the states $(n, m) = (0, 0)$, $(0, 1)$ and $(1, 0)$ in the case of a two-dimensional quadratic potential. The single-particle energy for the same states is shown in Fig. 4. Similar results are obtained for $d = 1$ and $d = 3$.

Figures 1-4 allow us to emphasize a possibly important consequence of the above conjecture. In the case $U_0 < 0$, the node-less solution exists only for $\mu < \mathcal{E}_0$. Therefore, in the range $\mathcal{E}_0 < \mu < \mathcal{E}_1$ the state with minimal energy is Ψ_1. This implies that controlling the chemical potential it is possible to obtain a condensate with a node or a vortex in the ground state.

3 The strongly non linear limit

The conjecture discussed so far concerned the behaviour of the solutions of Eq. (4) in the linear limit. An approximate expression of the solutions of (4) is possible also in the opposite limit $|\mu| \to \infty$. Let us consider first the case $U_0 > 0$. The repulsive interaction tends to delocalize the solutions so that the Thomas-Fermi approximation holds [15, 16]. In this case the gradient

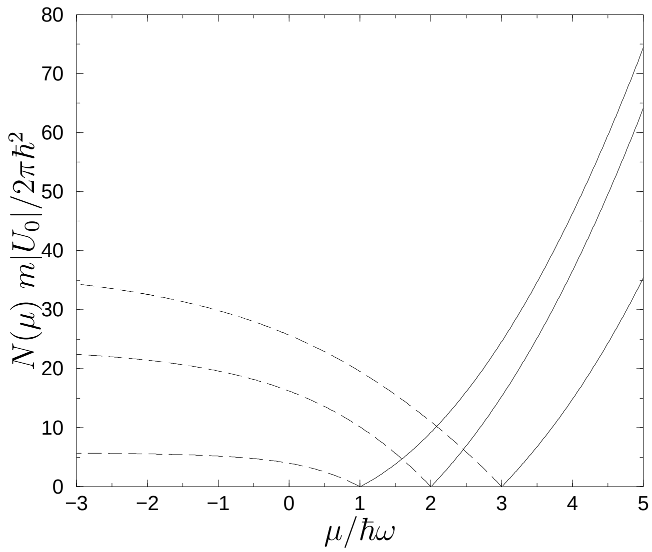

Figure 3: Number of particles N as a function of the chemical potential μ for a two dimensional quadratic potential. Solid and dashed lines are obtained by the solving numerically Eq. (4) for $U_0 > 0$ and $U_0 < 0$, respectively. The three curves correspond to the states $(n, m) = (0, 0)$, $(0, 1)$ and $(1, 0)$.

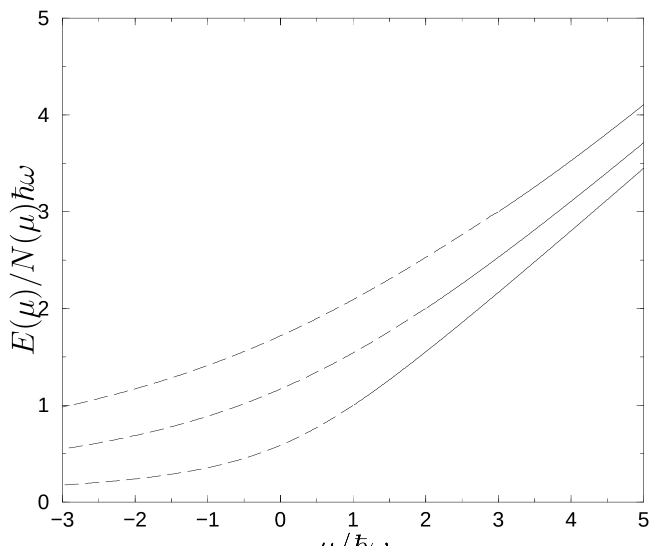

Figure 4: Single-particle energy E/N as a function of the chemical potential μ for the same states of Fig. 3.

term in Eq. (4) can be neglected and ψ is determined by

$$U_0|\psi(\boldsymbol{x})|^2\psi(\boldsymbol{x}) + V(\boldsymbol{x})\psi(\boldsymbol{x}) - \mu\psi(\boldsymbol{x}) = 0. \tag{33}$$

Therefore the ground state solution can be approximated as

$$\psi_0(\boldsymbol{x}) = \begin{cases} \sqrt{(\mu - V(\boldsymbol{x}))/U_0} & \mu > V(\boldsymbol{x}) \\ 0 & \mu < V(\boldsymbol{x}) \end{cases} . \tag{34}$$

In the one-dimensional case, n-node solutions may be approximated by a chain of dark solitons

$$\psi_n(x) = \psi_0(x) \prod_{k=1}^{n} \tanh\left(\frac{\sqrt{m\mu}}{\hbar}(x - x_k)\right) \tag{35}$$

with x_k to be determined, for instance by extremizing the functional Ω.

In the case of a quadratic potential the number of particles and the energy for the state (34) are

$$N(\mu) = \frac{2^{\frac{d+2}{2}}}{d(d+2)}\Lambda(d)\ \frac{\mu^{\frac{d+2}{2}}}{m^{\frac{d}{2}}U_0\omega^d}, \tag{36}$$

$$E(\mu) = N\mu\ \left(1 - \frac{2}{d+4}\right), \tag{37}$$

where $\Lambda(d)$ is the volume of the unitary d-dimensional sphere. From Eq. (36) we see that N diverges for $\mu \to \infty$. Similar results are obtained for other potentials.

In the attractive case $U_0 < 0$, the solutions of (4) tend to localize and the Thomas-Fermi approximation fails [15]. In this case, however, for $\mu \to -\infty$ the potential term $V\psi$ becomes negligible and Eq. (4) can be approximated as

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x}) + U_0|\psi(\boldsymbol{x})|^2\psi(\boldsymbol{x}) - \mu\psi(\boldsymbol{x}) = 0. \tag{38}$$

Recently numerical evidence has been provided that the number of particles confined in a two dimensional harmonic potential is limited in the case of attractive interaction [7]. This fact can be analytically understood from (38). With the change

$$\boldsymbol{x} = \frac{\hbar}{\sqrt{-m\mu}}\,\boldsymbol{\xi} \tag{39}$$

$$\psi(\boldsymbol{x}) = \sqrt{\frac{\mu}{U_0}}\ \phi(\boldsymbol{\xi}), \tag{40}$$

Eq. (38) can be rewritten in the adimensional form

$$-\frac{1}{2}\nabla^2_{\boldsymbol{\xi}}\phi(\boldsymbol{\xi}) - |\phi(\boldsymbol{\xi})|^2\phi(\boldsymbol{\xi}) + \phi(\boldsymbol{\xi}) = 0. \tag{41}$$

Note that in the one-dimensional case, n-node solutions may be approximated by a chain of bright solitons

$$\psi_n(x) = \sqrt{\frac{2\mu}{U_0}}\ \sum_{k=0}^{n}(-1)^k \text{sech}\left(\frac{\sqrt{-2m\mu}}{\hbar}(x - x_k)\right) \tag{42}$$

with x_k to be determined, for instance by extremizing the functional Ω. The number of particles corresponding to a solution of (41) is given by

$$\begin{aligned} N(\mu) = \int |\psi(\boldsymbol{x})|^2 d\boldsymbol{x} &= \frac{\mu}{U_0}\frac{\hbar^d}{(-m\mu)^{\frac{d}{2}}}\int |\phi(\boldsymbol{\xi})|^2 d\boldsymbol{\xi} \\ &= \frac{\hbar^d}{m^{\frac{d}{2}}|U_0|}|\mu|^{\frac{2-d}{2}}\Gamma_2(d), \end{aligned} \tag{43}$$

where $\Gamma_k(d) = \int |\phi(\boldsymbol{\xi})|^k\ d\boldsymbol{\xi}$ is a numerical constant. Therefore we have

$$\lim_{\mu\to-\infty} N(\mu) = \begin{cases} \infty & d = 1 \\ \frac{\hbar^2}{m|U_0|}\Gamma_2(2) & d = 2 \\ 0 & d \geq 3 \end{cases}. \tag{44}$$

In Fig. 5 we show the behaviour of $N(\mu)$ in the ground state obtained by solving numerically Eq. (4) with a harmonic potential in the cases $d = 1, 2, 3$. We have chosen the following realistic values for the parameters: $m = 3.818 \times 10^{26}$ Kg, $\omega = 10.0$ Hz and, for $d = 3$, $U_0 = 4\pi\hbar^2 a_s/m$ with $a_s = 2.75 \times 10^{-9}$ m [17]. For $d = 2$ and $d = 1$ we set $U_0 = 4\pi\hbar^2 a_s/mL$ and $U_0 = 4\pi\hbar^2 a_s/mL^2$ with $L = 10^{-5}$ m and $L^2 = 9 \times 10^{-10}$ m^2. The numerical results compare very well with the analytical approximations (36) for $U_0 > 0$ and (43) for $U_0 < 0$, respectively. In the case of Eq. (43), $\Gamma_2(d)$ has been evaluated numerically. We have $\Gamma_2(1) = 2.82842$, $\Gamma_2(2) = 5.85044$ and $\Gamma_2(3) = 6.68118$. Note that for $d = 3$, $N(\mu)$ has a maximum and vanishes for both $\mu \to -\infty$ and $\mu \to 3/2\hbar\omega$. This implies that the function $\mu(N)$ is not single-valued but has two branches in agreement with [18].

In Fig. 6 we show the single-particle energy evaluated numerically in the same cases of Fig. 5. For $\mu \to \infty$ the energy diverges for any value of d according to the limiting expression (37). For $\mu \to -\infty$ the behaviour of $E(\mu)$ is well described by

$$E(\mu) = N\mu\ \left(1 - \frac{1}{2}\frac{\Gamma_4(d)}{\Gamma_2(d)}\right) \tag{45}$$

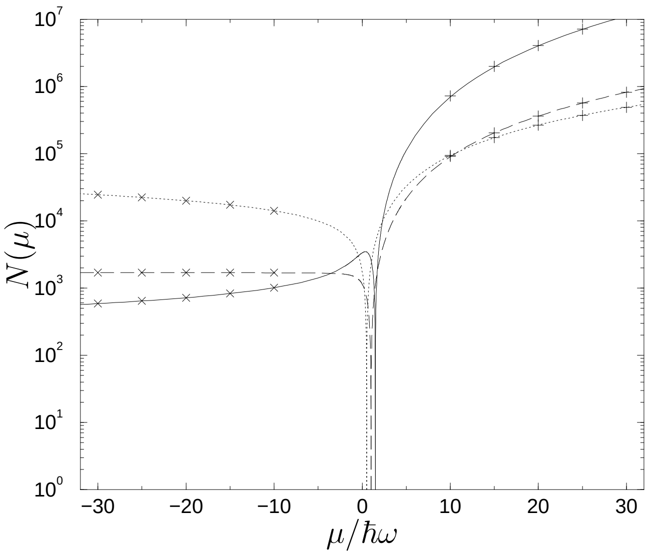

Figure 5: Number of particles N as a function of the chemical potential μ in the ground state of a quadratic potential with $d = 1$ (dotted line), $d = 2$ (dashed line) and $d = 3$ (solid line). The dots $+$ and $\times$ are the analytical results (36) and (43), respectively.

which easily stems from Eq. (41). For $d = 2$ we have $\Gamma_4 = 2\Gamma_2$ and hence $E(\mu)$ vanishes for $\mu \to -\infty$.

A Existence of a node-less state

In the following we suppose that the external potential is bounded from below and, for simplicity, we take $V(\boldsymbol{x}) \geq 0$. We will prove that, with $U_0 > 0$, a solution of (4) exists if and only if $\mu > \mathcal{E}_0$. The proof of the necessary condition is based on the property (6). Let us define the functional

$$Q_0[\psi] \equiv \int \left[\frac{\hbar^2}{2m} |\nabla \psi(\boldsymbol{x})|^2 + (V(\boldsymbol{x}) - \mu) |\psi(\boldsymbol{x})|^2 \right] d\boldsymbol{x}. \tag{46}$$

We have $\Omega[\psi] = Q_0[\psi] + \frac{1}{2} U_0 \int |\psi(\boldsymbol{x})|^4 d\boldsymbol{x}$. If $Q_0[\psi] > 0$, then $\psi(\boldsymbol{x})$ cannot be a solution of (4). The linear problem $Q_0'[\phi_n; \boldsymbol{x}] = k_n \phi_n(\boldsymbol{x})$, where

$$Q_0'[\phi_n; \boldsymbol{x}] \equiv \frac{\delta Q_0[\phi_n]}{\delta \phi_n(\boldsymbol{x})^*} = -\frac{\hbar}{2m} \nabla^2 \phi_n(\boldsymbol{x}) + (V(\boldsymbol{x}) - \mu)\, \phi_n(\boldsymbol{x}), \tag{47}$$

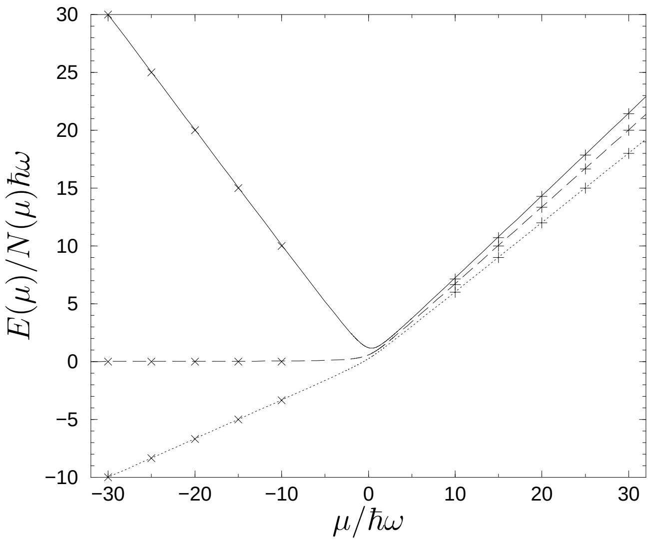

Figure 6: Single-particle energy E/N as a function of μ in the ground state of a quadratic potential with $d = 1$ (dotted line), $d = 2$ (dashed line) and $d = 3$ (solid line). The dots $+$ and $\times$ are the analytical results (37) and (45), respectively.

has the same eigenfunctions of (7) and the eigenvalues are $k_n = \mathcal{E}_n - \mu$. By decomposing a generic $\psi(\boldsymbol{x})$ as $\psi(\boldsymbol{x}) = \sum_{n=0}^{\infty} c_n \phi_n(\boldsymbol{x})$, we obtain

$$\begin{aligned} Q_0[\psi] &= (Q_0'[\psi;\boldsymbol{x}], \psi(\boldsymbol{x})) \\ &= \left(\sum_{n=0}^{\infty} c_n k_n \phi_n(\boldsymbol{x}), \sum_{m=0}^{\infty} c_m \phi_m(\boldsymbol{x}) \right) \\ &\geq k_0 \sum_{n=0}^{\infty} |c_n|^2. \end{aligned} \tag{48}$$

Therefore, if $\mu < \mathcal{E}_0$ we have $k_0 > 0$ and $Q_0[\psi] > 0$.

The sufficient condition can be proved with the help of general theorems on elliptic differential equations [19]. First we look for upper and lower solutions of (4). An upper solution $\psi_u(\boldsymbol{x})$ is defined by

$$-\frac{\hbar^2}{2m}\nabla^2\psi_u(\boldsymbol{x}) + U_0|\psi_u(\boldsymbol{x})|^2\psi_u(\boldsymbol{x}) + (V(\boldsymbol{x}) - \mu)\psi_u(\boldsymbol{x}) \geq 0. \tag{49}$$

For a lower solution $\psi_l(\boldsymbol{x})$ the inequality is reversed. If a couple of ordered upper and lower solutions exist, *i.e.* $\psi_u > \psi_l$, then the existence of, at least, one solution $\psi(\boldsymbol{x})$ with $\psi_l \leq \psi \leq \psi_u$ is guaranteed [19]. It is simple to check

that an upper solution is $\psi_u(\boldsymbol{x}) = \sqrt{\mu/U_0}$. As a lower solution we choose $\psi_l(\boldsymbol{x}) = \epsilon\phi_0(\boldsymbol{x})$ with

$$\epsilon < \min\left(\sqrt{\frac{\mu - \mathcal{E}_0}{U_0 \max_{\boldsymbol{x}} |\phi_0(\boldsymbol{x})|^2}}, \frac{\sqrt{\mu}}{\sqrt{U_0} \max_{\boldsymbol{x}} |\phi_0(\boldsymbol{x})|}\right) \tag{50}$$

which ensures that $\psi_l < \psi_u$.

In the case $U_0 < 0$, it is possible to prove that a positive solution of (4) does not exist if $\mu > \mathcal{E}_0$. Multiplying (4) by $\phi_0(\boldsymbol{x})$ and integrating, we have

$$\begin{aligned} 0 &= \int \phi_0(\boldsymbol{x}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U_0|\psi(\boldsymbol{x})|^2 + (V(\boldsymbol{x}) - \mu)\right] \psi(\boldsymbol{x})\ d\boldsymbol{x} \\ &= \int \psi(\boldsymbol{x}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U_0|\psi(\boldsymbol{x})|^2 + (V(\boldsymbol{x}) - \mu)\right] \phi_0(\boldsymbol{x})\ d\boldsymbol{x} \\ &= \int \psi(\boldsymbol{x}) \left[U_0|\psi(\boldsymbol{x})|^2 + (\mathcal{E}_0 - \mu)\right] \phi_0(\boldsymbol{x})\ d\boldsymbol{x}. \end{aligned} \tag{51}$$

Therefore,

$$U_0 \int \phi_0(\boldsymbol{x})|\psi(\boldsymbol{x})|^2\psi(\boldsymbol{x})d\boldsymbol{x} = (\mu - \mathcal{E}_0) \int \phi_0(\boldsymbol{x})\psi(\boldsymbol{x})d\boldsymbol{x}. \tag{52}$$

If $\psi(\boldsymbol{x})$ is a positive function, both integrals in (52) are positive and for $\mu > \mathcal{E}_0$ the equality is impossible.

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